Isobutyl methyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, isobutyl methyl ester
Inchi: InChI=1S/C13H16O4/c1-9(2)8-17-13(15)11-7-5-4-6-10(11)12(14)16-3/h4-7,9H,8H2,1-3H
InchiKey: HRJOMMSRROBCMQ-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: COC(=O)c1ccccc1C(=O)OCC(C)C
Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	-308.92	kJ/mol	Joback Method
hf	-581.47	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.286		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
tb	680.64	K	Joback Method
tc	893.11	K	Joback Method
tf	404.53	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.10	J/mol×K	680.64	Joback Method
cpg	502.29	J/mol×K	716.05	Joback Method
cpg	515.58	J/mol×K	751.46	Joback Method
cpg	527.98	J/mol×K	786.88	Joback Method
cpg	539.49	J/mol×K	822.29	Joback Method
cpg	550.12	J/mol×K	857.70	Joback Method
cpg	559.87	J/mol×K	893.11	Joback Method

dvisc	0.0012327	Pa×s	404.53	Joback Method
dvisc	0.0006913	Pa×s	450.55	Joback Method
dvisc	0.0004315	Pa×s	496.57	Joback Method
dvisc	0.0002918	Pa×s	542.59	Joback Method
dvisc	0.0002097	Pa×s	588.60	Joback Method
dvisc	0.0001582	Pa×s	634.62	Joback Method
dvisc	0.0001239	Pa×s	680.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume